

ACP Facilities: Gulfstream 159 and Wiley EMSL

**Atmospheric Chemistry Program Facilities:
Gulfstream 159 Research Aircraft
and
W. R. Wiley Environmental Molecular Sciences
Laboratory**

**W.R. Barchet
Pacific Northwest National Laboratory
June 23, 1999**

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DOE Research Aircraft Facility



Grumman Gulfstream 159 (G-1) twin turboprop aircraft

DOE Research Aircraft Facility

- **A DOE/OBER/ESD resource for atmospheric chemistry research**
- **Instrument development, testing, and application; field study support**
- **Up to 250 flight hours per year**
- **Requests for access reviewed and recommended by Advisory Panel**

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Attributes of the G-1 Research Aircraft



- **Dimensions:** Length 20 m, Wingspan 24 m, Height 21 m, Weight 16,330 kg max
- **Nominal operation:** Altitude 0.5-7.5 km, Cruise speed 80-200 m/s, Sampling speed 100 m/s, Climb 160-330 m/min
- **Endurance with maximum fuel:** 6 hr
- **Power:** 4,000 VA @ 115&230 VAC, 28 VDC
- **Crew:** 2 pilots, 1-4 scientists
- **Cabin payload:** 1,300 kg

Instrumentation on G-1

- Meteorological sensors
 - Temperature, pressure, dew point temperature
 - Gust probe vector winds
- Chemical sensors
 - Real-time: O_3 , CO , SO_2 , NO/NO_2 , H_2O , H_2O_2
 - Integrating: filter pack (SO_2 , SO_4 , NO_3 , HNO_3 , NH_4), PAN, VOC



Gust Probe Ports

Instrumentation on G-1

(continued)



- **Cloud & Aerosol Microphysics**
 - PMS PCASP, FSSP, 2D aerosol/cloud size spectra
 - Total scatter/back scatter nephelometers
 - Condensation particle counter
 - Ultrafine particle counter
 - Liquid water content
- **Radiation**
 - UV/solar/IR radiometers
 - Up/down-looking IR thermometers

Instrumentation on G-1

(continued)

- External instrumentation collaboration
 - BNL: NO_x/NO_y , H_2O_2 , Carbonyl
 - BCO: API-MS, PAN-GC, VOC
 - ANL: VOC, VOC-GC, NO_2 /PAN
 - U-WA: CFVI, CCN, B_{scat}
 - U-NV/DRI: CCN spectrometer
 - PNNL: ITMS, Radionuclide collector



BCO API 365 MS/MS

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Instrumentation on G-1
(continued)



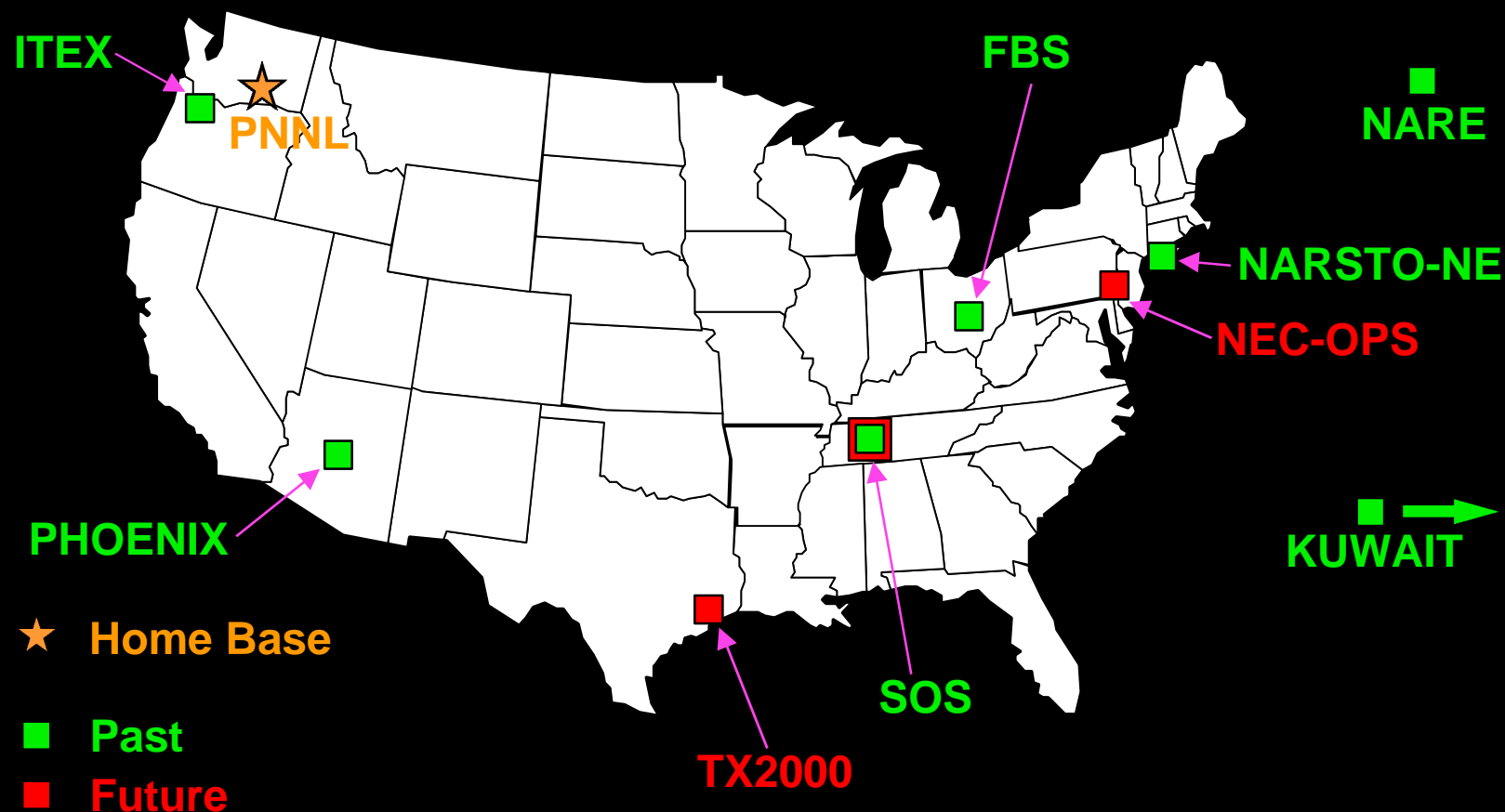
View aft



View forward

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***Locations of ACP Projects Using
the DOE RAF G-1***



Requests for DOE RAF Use

- Requests are submitted to a review panel for evaluation
- DOE authorizes flight time
- Priority given to DOE/OBER/ESD projects
- Contact W. R. Barchet for more information or application for flight hours:
e-mail: **rich.barchet@pnl.gov**
phone: **509-372-6158**
fax: **509-372-6168**

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W. R. Wiley
Environmental Molecular Sciences Laboratory

- **Tour of the EMSL Laboratory**
- **Examples of Research Directed at Atmospheric Sciences Needs**

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Mission

- . . . provide the fundamental scientific basis needed to solve the nation's environmental problems.**
- . . . advance molecular science in support of the long-term missions of the U.S. Department of Energy.**

National Scientific User Facility

- . . . make unique research resources available to DOE scientists and researchers from academia and industry.**
- . . . provide opportunities needed to educate and recruit young scientists to meet the demanding environmental challenges of the future.**

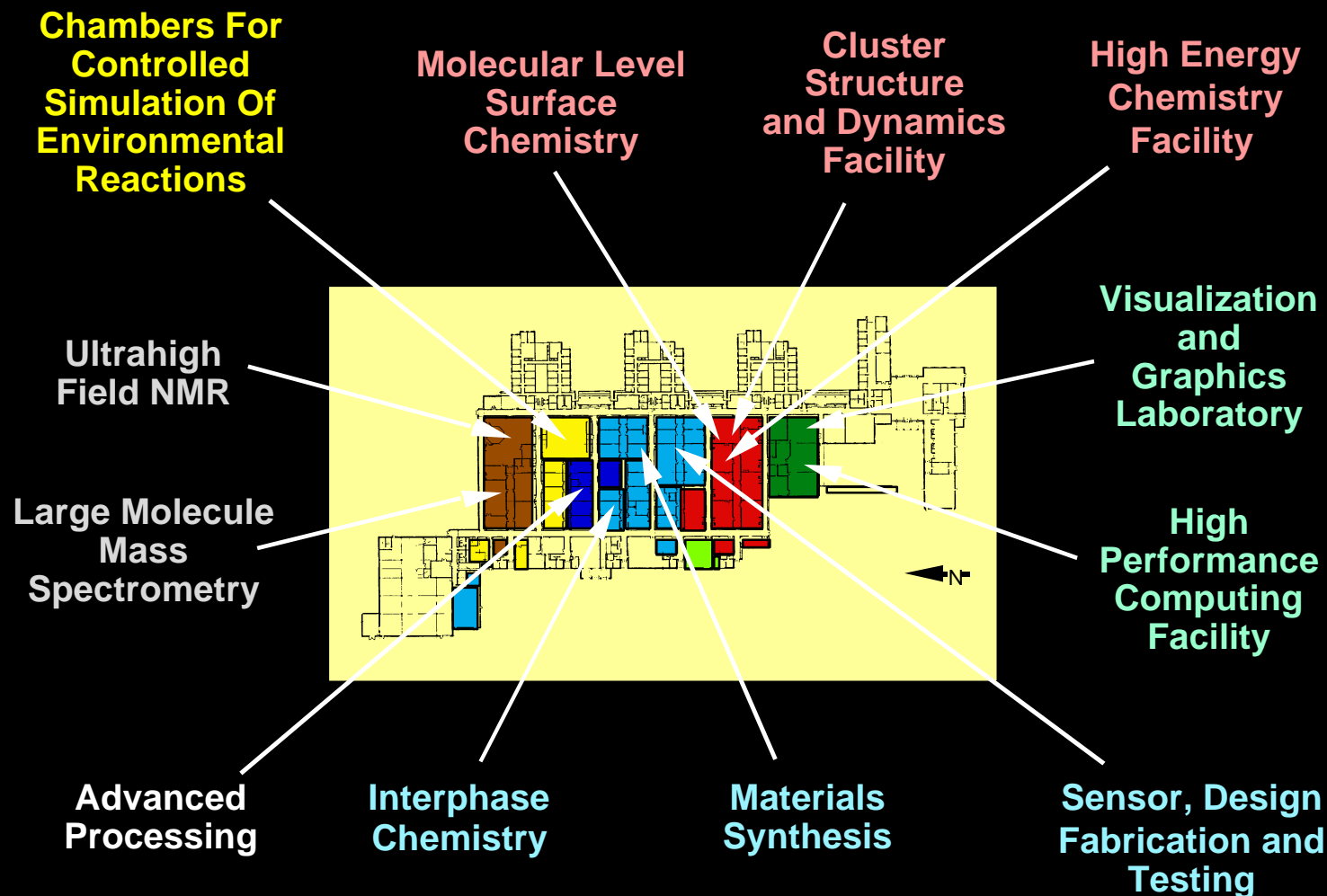
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Nature of the EMSL as a User Facility:

- Primary **Mission** is Environmental Molecular Science
- Equipment Available for Both **Collaborative and Independent** Use
- **Wide Range** of Capabilities Available Within One Facility
- Web Based Applications Judged by
 - Scientific Merit
 - Applicability of Proposed Use
 - Equipment/Staff Availability

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Advanced Research Capabilities for Environmental Molecular Science



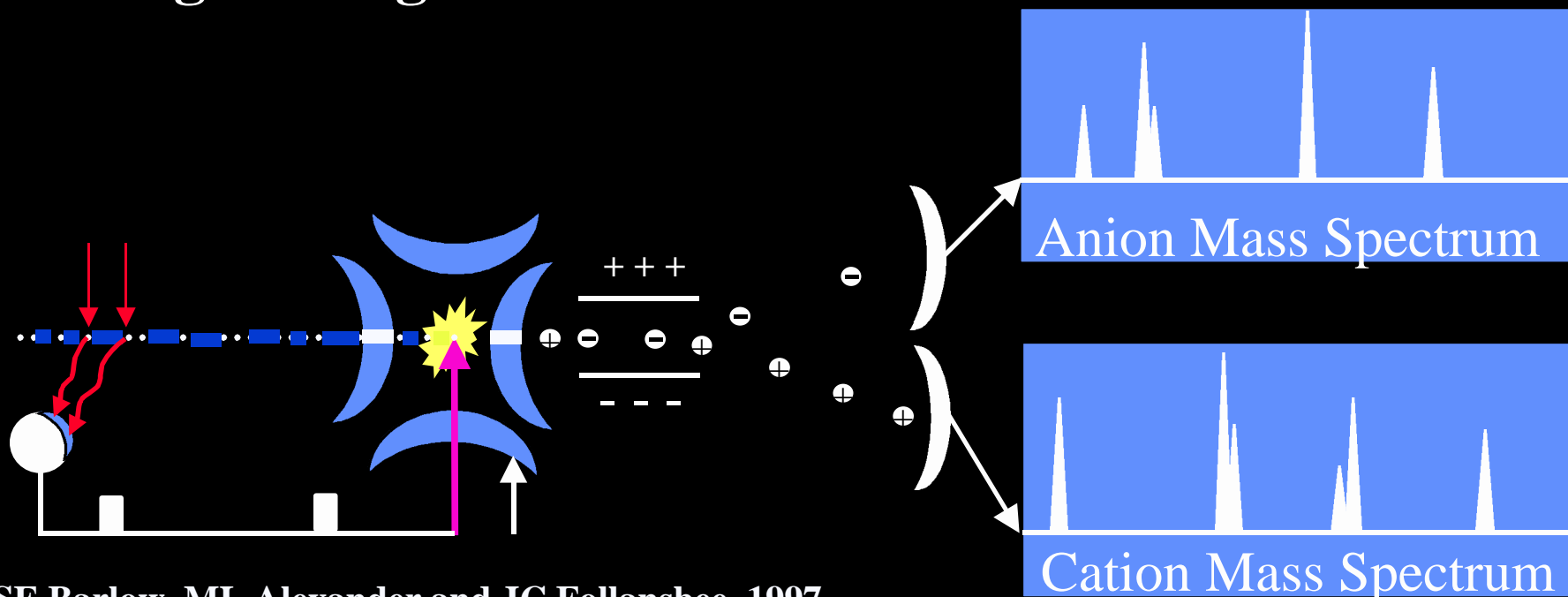
The High Field Mass Spectrometry Facility

- **World's first 11.5-tesla Fourier transform ion cyclotron resonance mass spectrometer**
- **State-of-the-art 7- tesla FTICR mass spectrometer**
- **Broad array of other mass spectrometers available for use**



Aerosol Mass Spectrometer

- **Asymmetric Ion Trap: Single Particle MS**
 - Mass M/Z of 10 amu to 650 amu with unit resolution
 - Simultaneous Anion/Cation Detection
 - Light Weight/Low Power - Portable

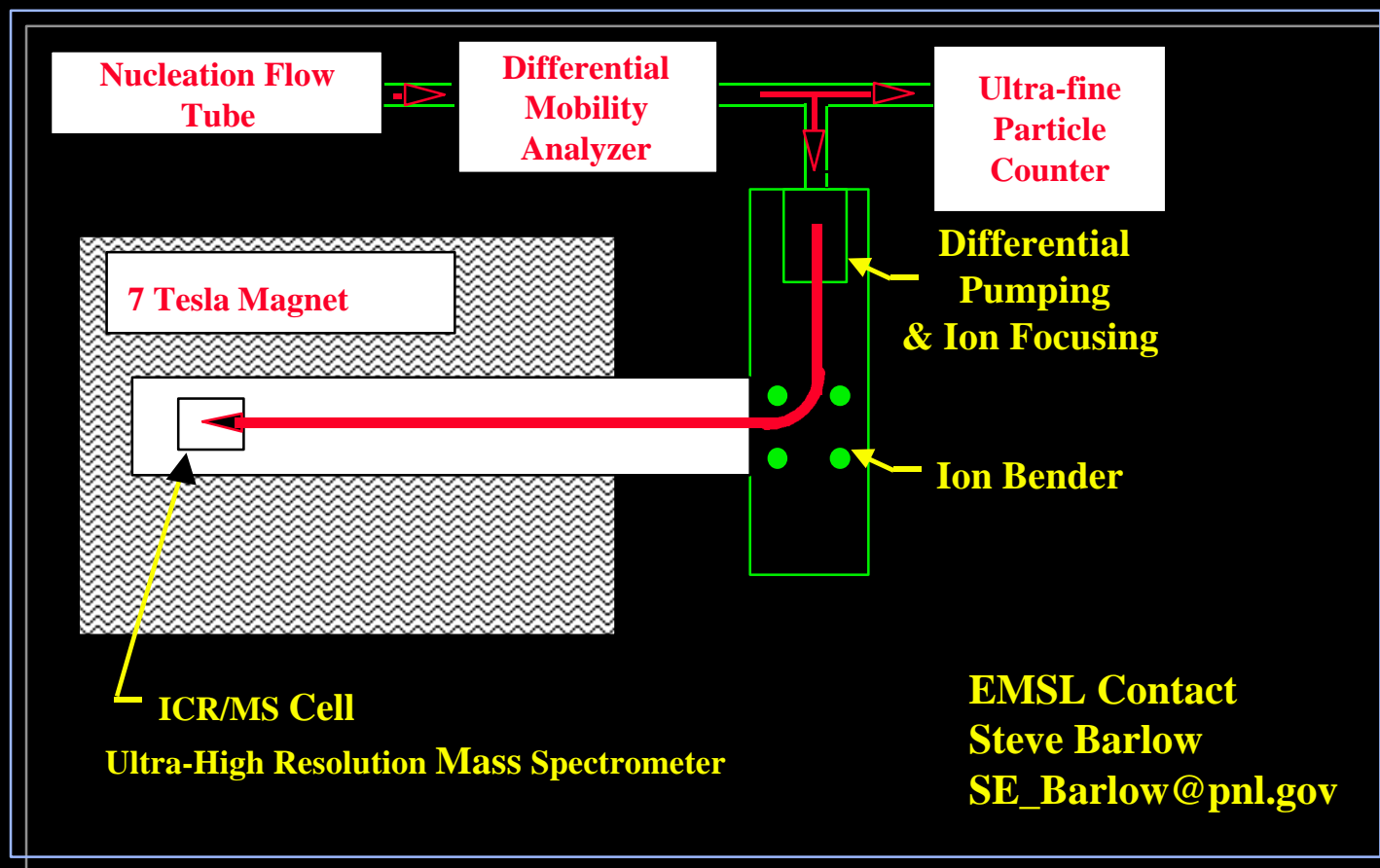


SE Barlow, ML Alexander and JC Follansbee, 1997

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Schematic of Aerosol Nucleation Experiment

Research to determine critical concentrations of trace gases, e.g., ammonia and/or nitric acid, that promote formation of condensation nuclei.



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The Molecular Science Computing Facility MSCF

- **512-processor IBM RISC System/6000 Scalable POWER parallel (IBM SP) computer system**
 - 67 gigabytes of memory
 - 2.9 terabytes of online disk
 - 20 terabyte EMASS storage
- **Graphics and visualization system**
 - High-performance Silicon Graphics
 - Integrated digital video and audio editing system
- **A new generation of molecular modeling software**
 - Electronic structure and molecular dynamics calculations



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Molecular Science Computing Facility

Supports:

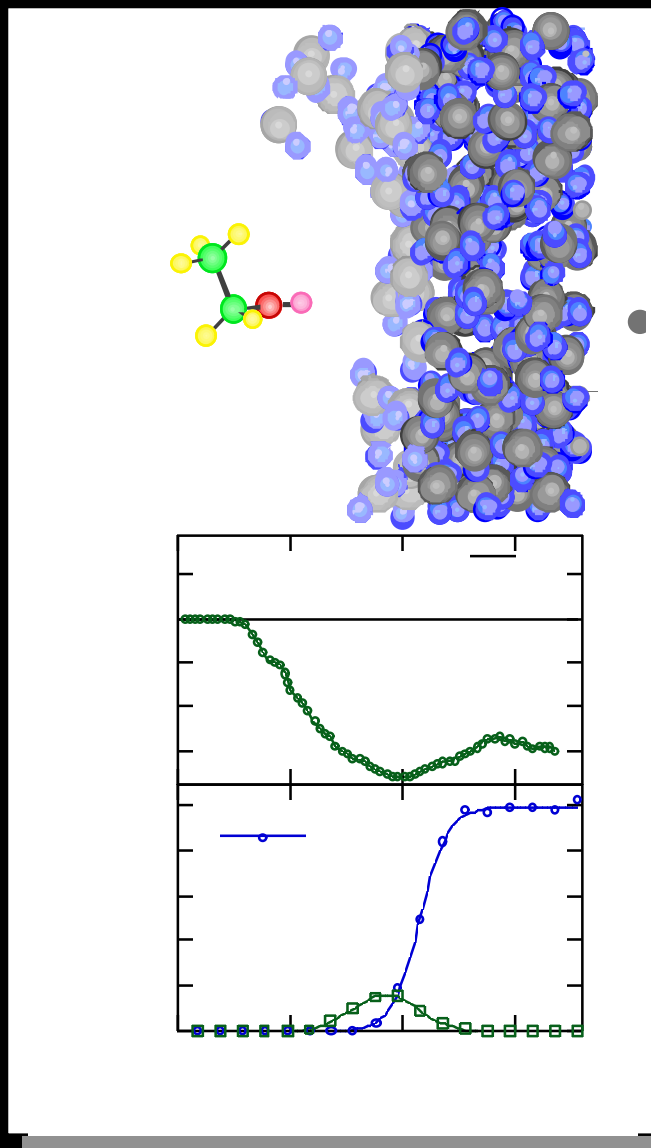
- benchmark calculations on small molecules
- reliable calculations on large molecules and solids
- simulations of large biomolecules
- reactive chemical transport modeling.

Includes: Hardware, software, associated support staff, and a user-support staff (2 to 3 consultants).

Access: Centered around the concept of “Computational Grand Challenge” teams.

EMSL Contact: Dave Dixon
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www.emsl.pnl.gov



Molecular Theory and Modeling

- Nucleation of Tropospheric Aerosols
- Molecular Dynamics Simulation of Uptake by Water Droplets

○ Potential of Mean Force

○ Water Density

□ Ethanol Density

EMSL Contact: Bruce Garrett
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***One Hundred Research Stations for
Environmental Molecular Sciences Research***

Nanostructural Materials - Design and synthesis of model materials.

Interfacial Structures and Compositions - Characterization of atomic and molecular structures, defect structures, and compositional variations across and through interfaces.

Reactions and Interfaces - Studies of chemical and physical processes at model and natural interfaces.

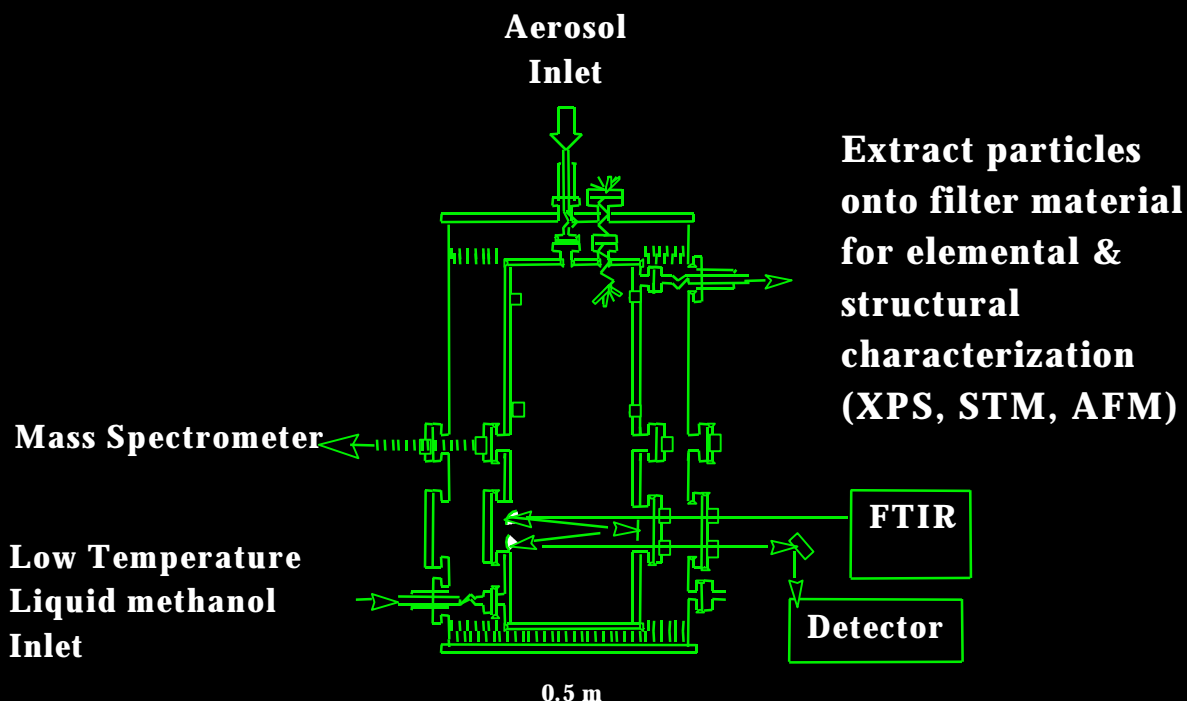
Gas-Phase Monitoring and Detection - Research in detection and monitoring of trace chemicals.

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Laboratory Studies of Atmospheric Heterogeneous Chemistry

Typical Research

- Obtain heterogeneous aerosol reaction efficiencies (carbonaceous soot, sea-salt, etc.) for use in atmospheric models.
- Identify interactions among trace gas species of atmospheric interest.
- Elucidate chemical mechanisms/rate processes.



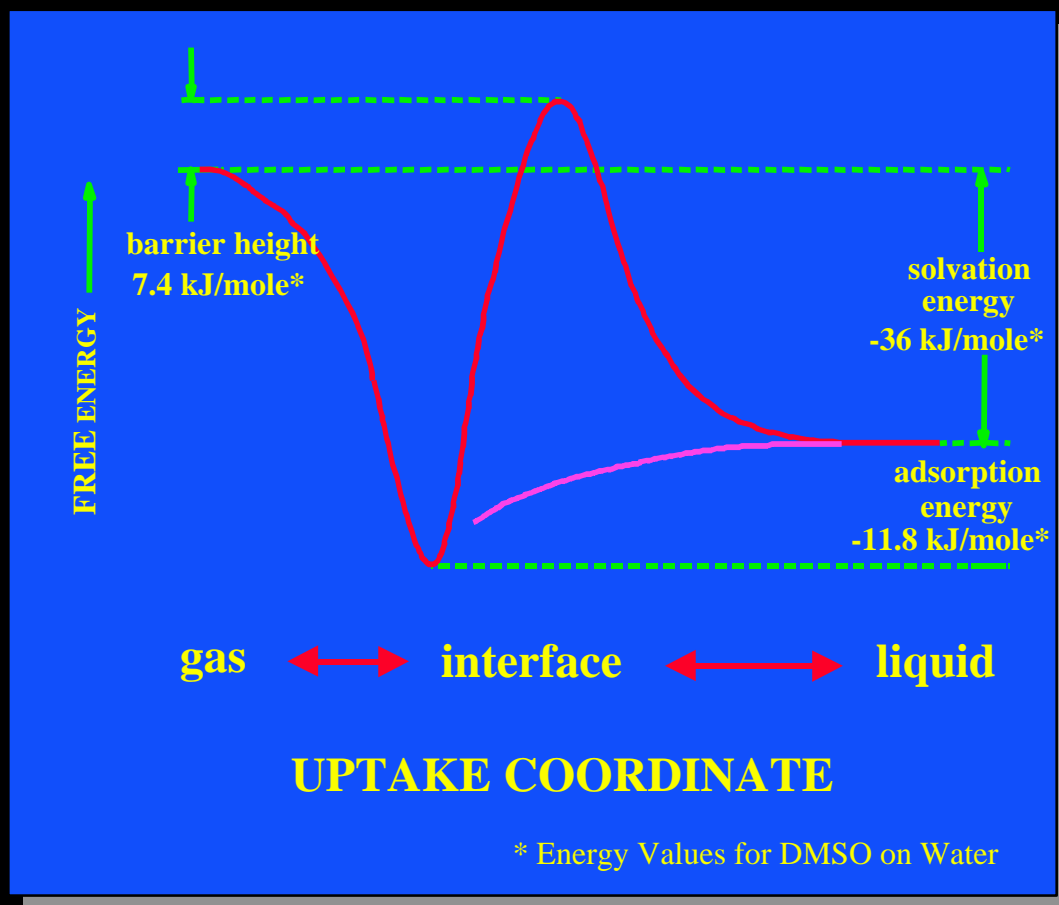
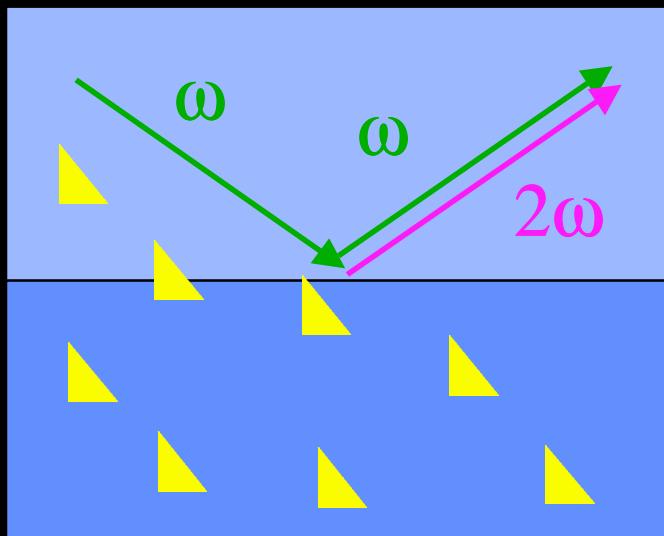
Aerosol Reactions Chamber

1. Temperature controlled from 300 to 185 K.
2. Teflon coated inner surfaces.

EMSL Contact
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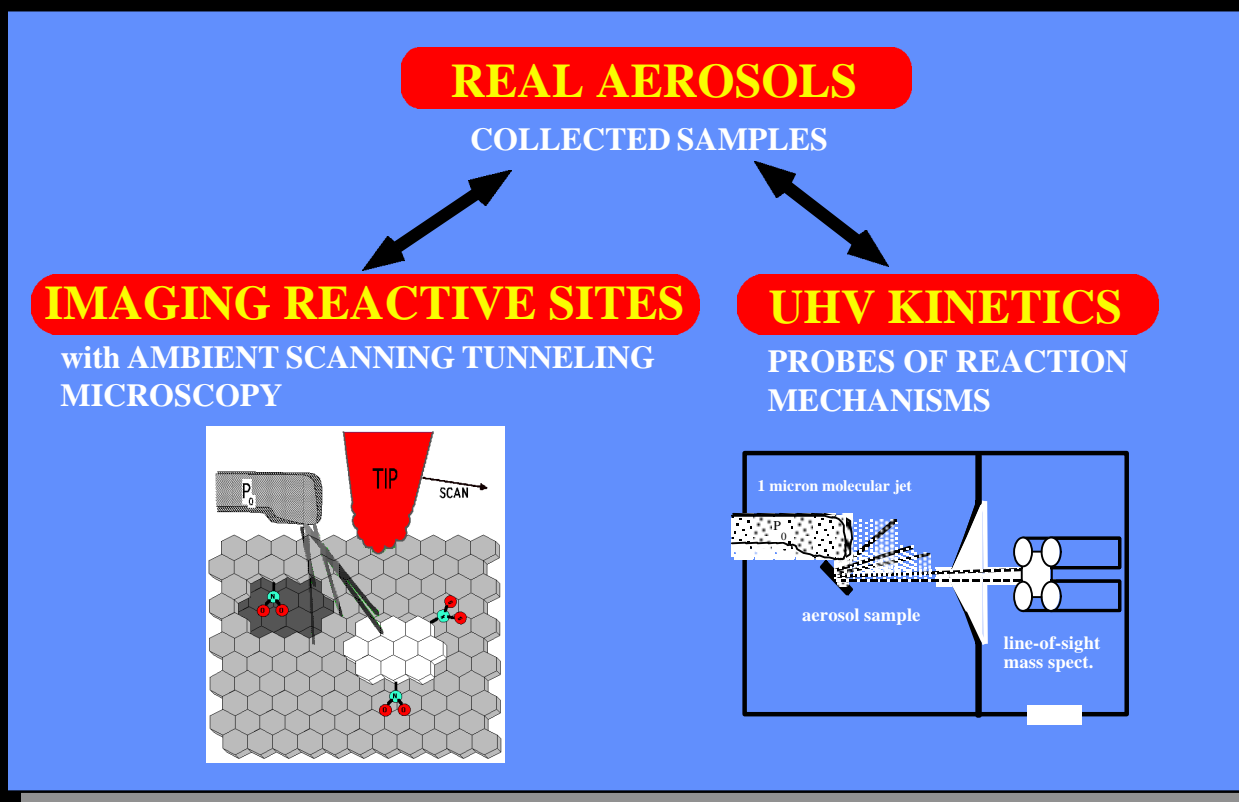
Surface Second Harmonic Generation Studies of Gas/Liquid Uptake Energetics



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D_Ray@pnl.gov

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***Combining Surface Characterization (AFM, STM, XPS,
With Molecular Jet Sources and Mass Spectroscopy to
Determine Reaction Mechanisms and Rates.***

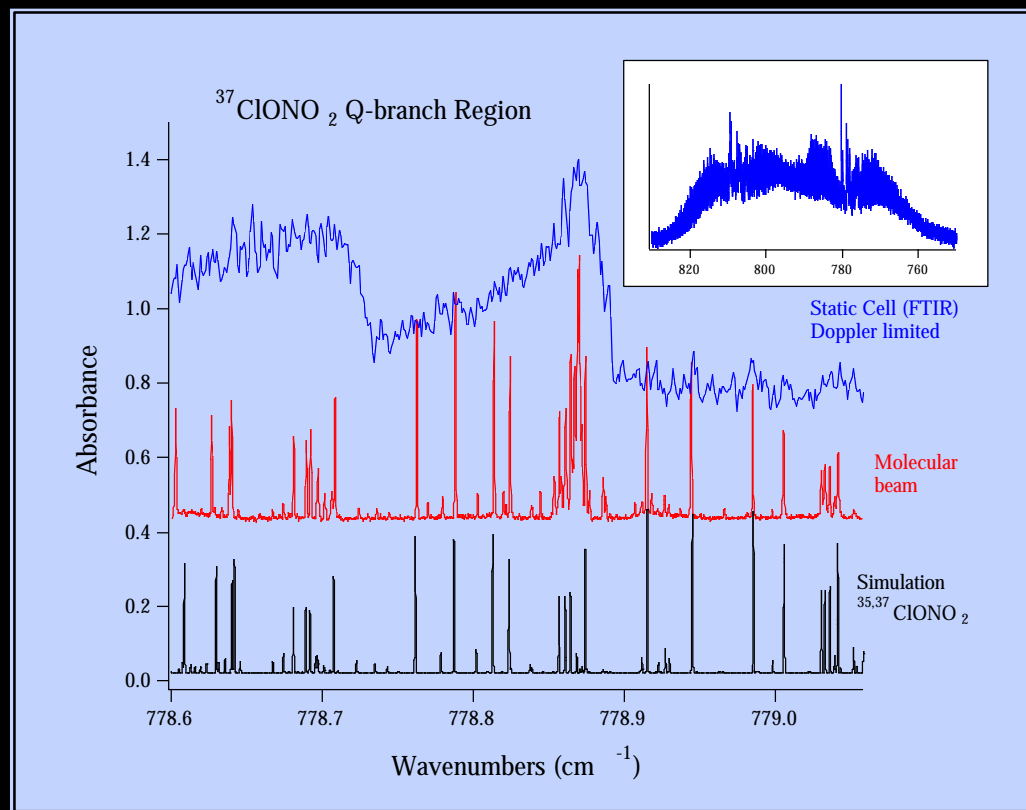


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Infrared Spectroscopy: In Cells, Jets & the Field

Current Research

- Laboratory measurements of the “atmospheric continuum”
- Development of laser-based sensors for trace atmospheric gasses
- Development of high resolution spectral database
- Ultra-cold molecular spectroscopy (5-10K)



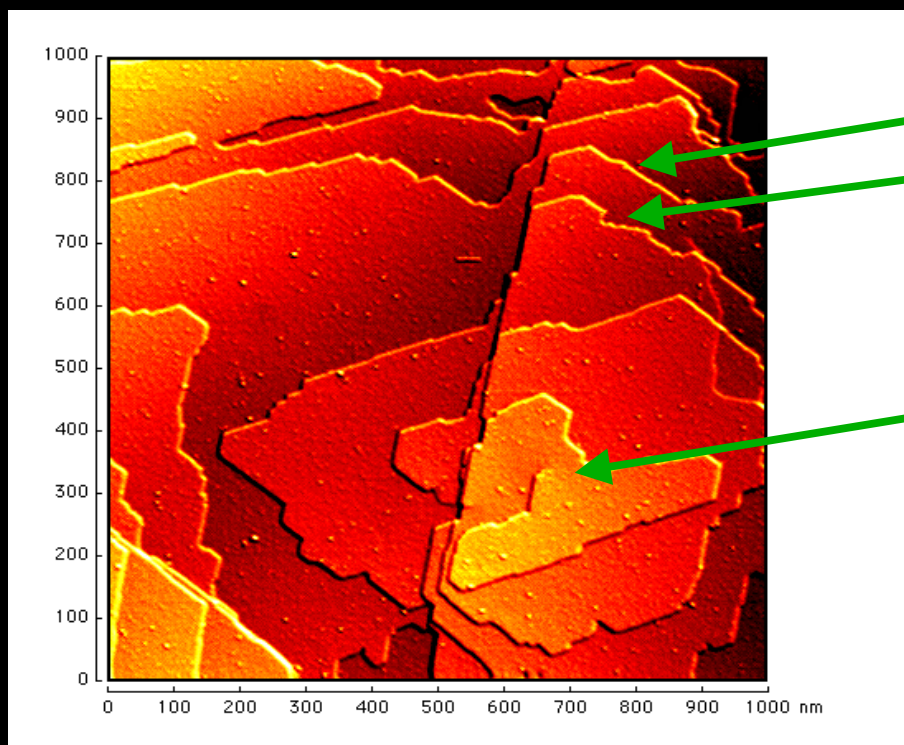
Ultra-cold gas phase spectroscopy

EMSL Contact: Steve Sharpe, SW_Sharpe@pnl.gov

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Atomic Resolution Surface Analysis of Aerosols

- Surface Topology Mapping
- Surface Chemical Analyses



**Atomic Height
Steps**

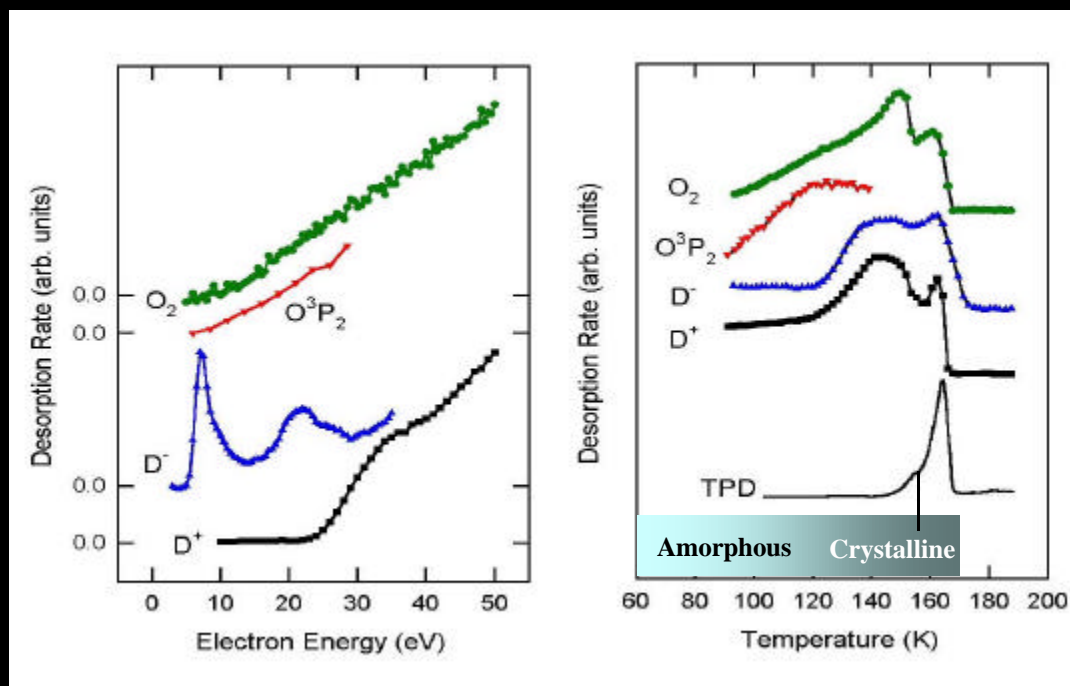
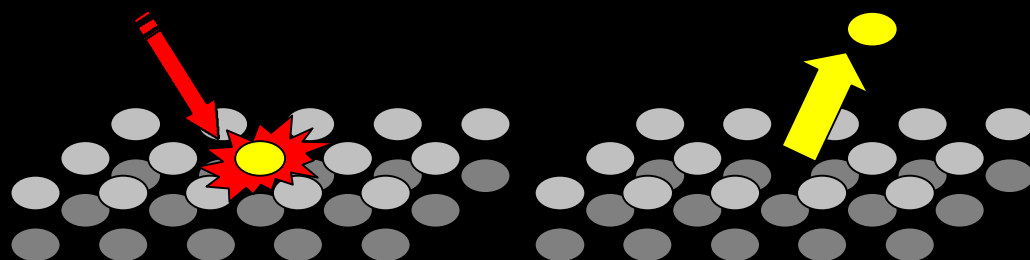
**Screw
Dislocation**

Scanning Tunneling Microscope Image of Natural $\alpha\text{-Fe}_2\text{O}_3(001)$ Surface

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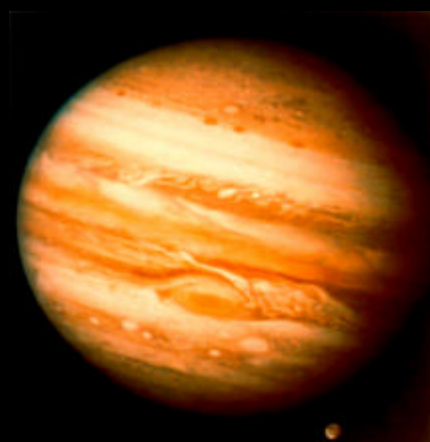
Understanding Radiochemistry and Plasma Chemistry:

Electron-Stimulated Desorption from D₂O Ice

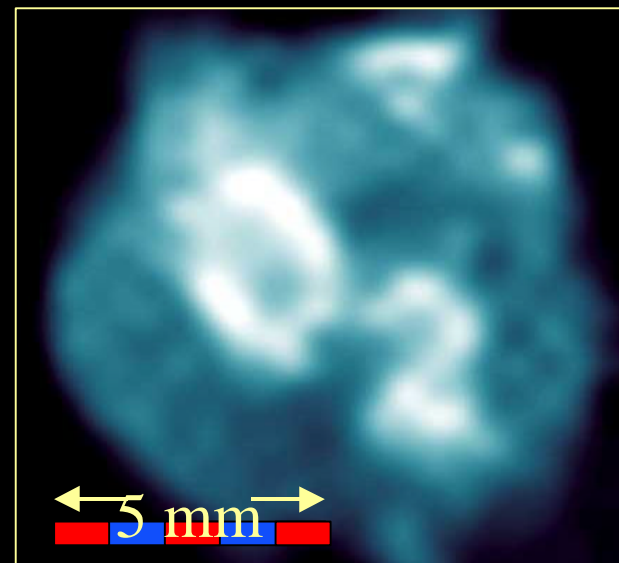
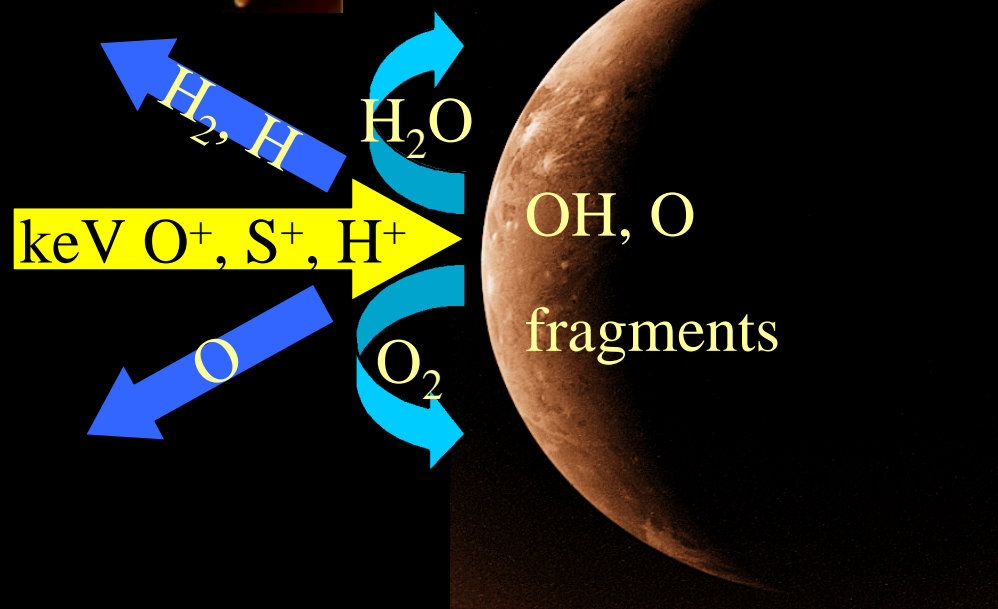


**Products change
with electron
energy and
water mobility**

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**Thin O₂ atmospheres
have been reported on
the Jovian moons
Ganymede and Europa.**



M. T. Sieger, W. C. Simpson, and T. M. Orlando, *Nature*, in press

Conducting Atmospheric Sciences Research

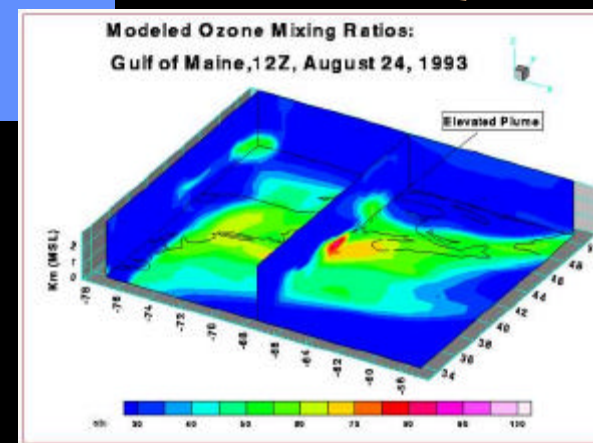
- **Team Effort Involving Many Disciplines**
- **Focused on National Needs**
 - *Air Quality: Oxidants, Particles*
 - *Understanding Global Change*
- **Model Based**
- **Requires Close Coupling of Programs**
 - *Operational Sensitivity Analysis*

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Operational Sensitivity Analysis



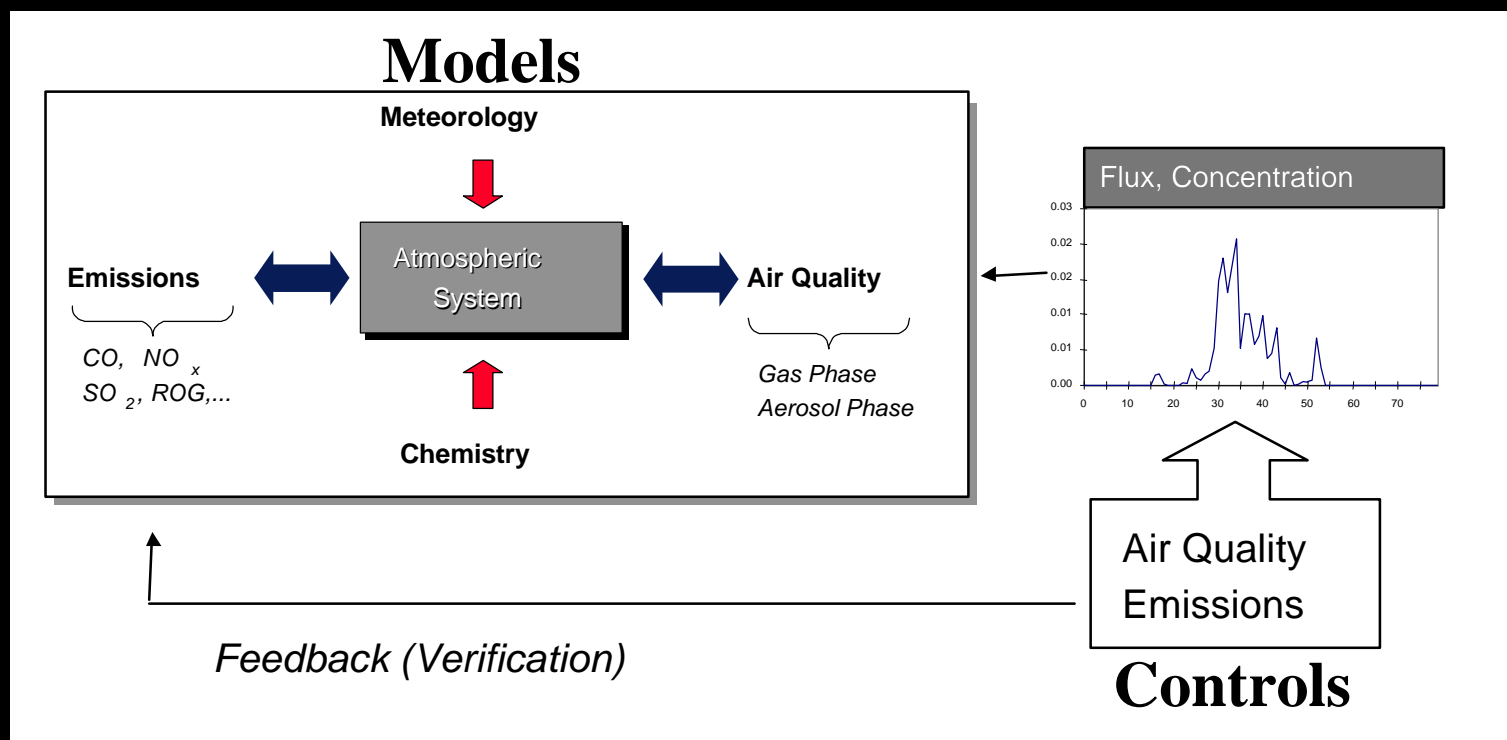
- Data Requests
- Results
- Surprises



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Models

- Relationship Between Controls and Air Quality
- Basis for Laboratory and Field Experiments



Gaining Access to the EMSL

- **Use The Web Based Information Resources and User Application: www.emsl.pnl.gov**
- **Contact an EMSL Staff Member (optional)**
i.e. Steve Colson at
email: SD_Colson@pnl.gov
phone: (509) 376-4598
FAX: (509) 376-0846